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Solute dispersion in a variably saturated sand

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[1] The understanding of solute dispersion in unsaturated porous media is still nascent. This work focuses on the measurement of solute dispersion in porous media at various levels of pore-volume saturation and on the parameterization of longitudinal dispersivity in terms of the saturation ratio and a soil's textural characteristics. The dispersion coefficient was determined in partly saturated columns packed with Toyoura sand or glass beads under steady state flow. A 0.0282 N sodium chloride solution was used as a nonreactive tracer in a series of laboratory experiments in which, for a fixed water content, the average pore-water velocity was varied. The column experiments showed that the dispersion coefficient increases linearly with increasing water velocity for a fixed water content and that the slope of the dispersion coefficient versus water velocity relationship diminishes as the water content is increased. The Peclet number (Pe) was fitted to the experimental tracer data by a nonlinear function $Pe = aS_r^b$, in which S_r is the saturation ratio and a and b are texture-dependent parameters. The dispersivity (α , in centimeters) of the test columns' porous media was then estimated in terms of the saturation ratio and the median grain size (d_{50} , in centimeters) by the power law $\alpha = d_{50}/Pe = d_{50}/aS_r^b$, which provides a specific functional relationship among a porous medium's dispersion properties, the saturation ratio, and the medium's textural characteristics. *INDEX TERMS:* 1829

Hydrology: Groundwater hydrology; 1831 Hydrology: Groundwater quality; 1832 Hydrology: Groundwater transport; 1875 Hydrology: Unsaturated zone; 1894 Hydrology: Instruments and techniques; *KEYWORDS:* unsaturated transport, solute dispersion, soil moisture, soil characteristic curve

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1. Introduction

[2] The objective of this study is to investigate the roles of pore-water velocity, water content, and soil textural properties on solute dispersion in unsaturated porous media. Several authors have examined the process of dispersion in fully saturated porous media [see, e.g., *Saffman*, 1959; *Scheidtger*, 1960; *Rumer*, 1962; *Bear*, 1972]. Their findings suggested a linear relationship between the longitudinal dispersion coefficient and the average pore-water velocity, at least for moderate water velocity. Other research has addressed dispersion phenomena in unsaturated soils. *Nielsen and Biggar* [1961], for example, reported the shape of a tracer's breakthrough curve in an unsaturated sand. *Krupp and Elrick* [1968] compared breakthrough curves in unsaturated and saturated glass beads. *Yule and Gardner* [1978], were, to our knowledge, the first to quantify the dispersion coefficient in unsaturated soil. They found that the dispersion coefficient was larger in unsaturated soils than that in saturated ones. In addition, the latter authors pointed out the

difficulty of isolating experimentally the effect of water velocity on dispersion at constant water content. *De Smedt and Wierenga* [1984] discussed breakthrough curves in unsaturated glass beads and concluded that preferential flow is an important feature of solute transport in unsaturated porous media. *Maraqa et al.* [1997] reported experimental results for dispersivity as a function of water saturation and considering the role of immobile water in sandy soil columns. *Wildenschild and Jensen* [1999] found that flow pathways in a system of randomly heterogeneous sand columns were dependent on the water content. *Haga et al.* [1999] proposed an empirical relationship between the Peclet number (Pe) and the saturation ratio (S_r) based on tracer experiments in glass-bead media. Their proposed equation took the form $Pe = aS_r^b$, in which a and b are experimental constants. *Padilla et al.* [1999] studied the role of water content on dispersivity using silica-sand columns. The latter authors concluded that an increase in the fraction of immobile water contributes to greater dispersivity in unsaturated flow, in agreement with the mobile-immobile transport model of *van Genuchten and Wierenga* [1976]. *Forrer et al.* [1999] investigated field-scale solute dispersion

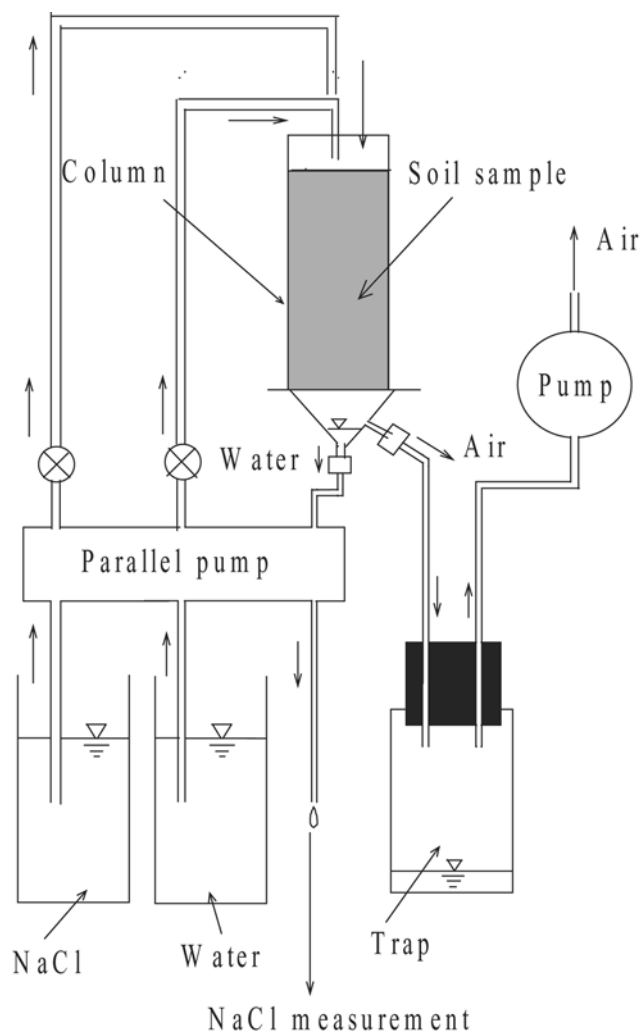


Figure 1. Experimental column system.

experimentally. Their research showed (1) that dispersion increased with decreasing water content and with increasing spatial variability of the water content, and (2) that the saturation-dependent nature of dispersion is influenced by the anisotropic transport properties of soils. *Gamerding and Kaplan* [2000] reported a centrifuge-based method to evaluate solute transport in unsaturated soil under steady state flow. Their experiments confirmed the increase in the dispersion coefficient with decreasing saturation ratio and with the increase in immobile water, whose fraction rises as the saturation ratio diminishes. In the realm of theoretical unsaturated dispersion analysis, *Mantoglou and Gelhar* [1985] derived an equation in which dispersivity was directly proportional to the variance of saturated hydraulic conductivity and inversely proportional to the mean pore size. Theirs was a stochastic analysis of longitudinal dispersion based on principles of mass conservation.

[3] There is an important difference in the experimental study of dispersion in saturated and unsaturated porous media as a function of pore-water velocity. In a saturated medium, the water velocity can be varied by manipulating the hydraulic gradient that drives flow through a column. In unsaturated porous media, on the other hand, a change in pore-water velocity is typically associated with a change

in its water content also. Thus a key challenge in the experimental study of dispersion in unsaturated soils is the ability to separate the effects of pore-water velocity and water content on dispersion, which this research addresses by means of novel experimental design. This article's objective is to further study the dependence of the dispersion coefficient on water content and pore-water velocity in unsaturated porous media. Previous research is expanded by considering the effect of soil texture on the dispersion versus water-content relationship.

2. Experimental Setup and Methods

2.1. The Test-Column System

[4] The test-column system is shown in Figure 1. The column has a 5-cm internal diameter and a length $L = 12$ cm. Tap water was pumped from a source and injected at the top of the column at a constant flow rate. Pore water was drained at the bottom of the column. After a steady state flow condition was established, a 0.0282N NaCl water solution was injected at the same flow rate at the top of the column. The solution water drained into a chamber collector where the chloride ion was measured by the Mohr method [*American Public Health Association (APHA)*, 1992]. The chloride (background) concentration (C_0) in tap water was measured similarly and used to establish the above-background chloride concentration (C) of the effluent water from the column.

[5] Controlled air suction was applied to the sample at the bottom of the column to suppress boundary effects and to keep a uniform water content throughout the column. The applied suction was measured with a manometer connected to a regulated air-suction pump. The magnitude of the applied suction necessary to achieve a desired saturation ratio for a given flow rate was determined from an experimentally derived flow-suction-saturation ratio curve shown in Figure 2. The flow rate corresponding to a specific suction

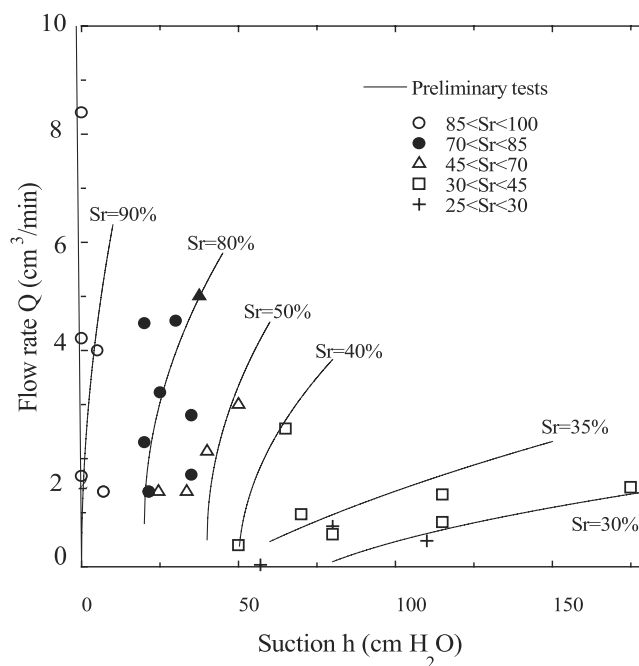


Figure 2. Suction/flow-rate/saturation-ratio curves in a Toyoura sand.

was determined by direct measurement of the effluent discharge and verified with a parallel pump. The column-wide saturation ratio was calculated as the average of individual measurements made on 3-cm (nonoverlapping) intervals of the porous medium within a column in a battery of column tests carried out to construct the diagrams depicted in Figure 2. The interplay of precisely controlled flow rate and suction application in conjunction with the diagrams shown in Figure 2 allowed us to study dispersion phenomena under variable flow rate, and thus variable average pore-water velocity at different levels of saturation ratio. The saturation ratio of each 3-cm interval was estimated by standard weighing and drying procedures. The vertical distribution of the saturation ratio within a column for fixed suction and flow rate was nearly constant, except for slightly larger values at the discharge (bottom) part of the column, where the suction was applied. A typical saturation-ratio profile is shown in Figure 3, in this case for an average velocity of 0.5 cm min^{-1} , which confirms the uniformity of the saturation ratio achieved along the test column.

2.2. Particle Size and Water-Retention Characteristics of the Test Media

[6] Toyoura sand and glass beads were used in the tracer experiments. Their water-retention characteristics were derived (as pore water was drained) using the suction plate

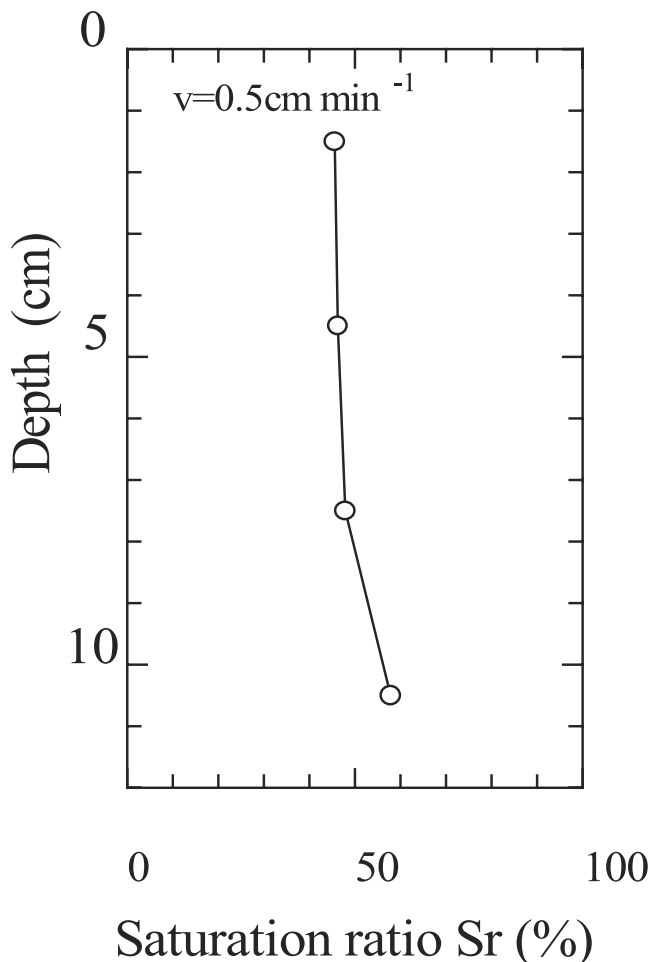


Figure 3. Saturation ratio in test column (average $S_r = 50\%$).

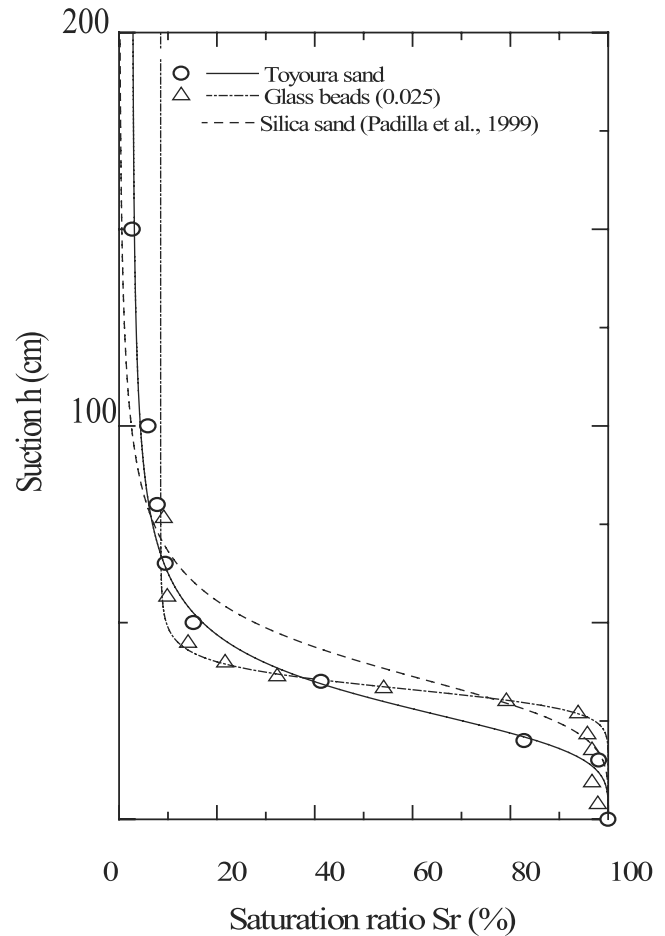


Figure 4. Water-retention characteristic curves for selected porous media (drainage process). Here $d_{50} = 0.025 \text{ cm}$ in glass beads.

method and are presented in Figure 4, which shows also the silica sand used by *Padilla et al.* [1999] and whose research results are relevant to our study. The *van Genuchten* [1980] α^* and n^* soil-moisture parameters as well as several grain-size indicators and particle densities were determined for the Toyoura sand, glass beads, and the silica sand and are shown in Table 1. The parameters α^* and n^* are related to the effective saturation ratio S_r by the following equation, in which h denotes soil-water tension (in centimeters):

$$S_r = \frac{1}{[1 + (\alpha^* h)^{n^*}]^{1/n^*}} \quad (1)$$

in which $S_r \equiv \theta - \theta_r / \theta_s - \theta_r$, θ is (volumetric) water content, and θ_r and θ_s are the residual water content and the water content at saturation, respectively. The parameters α^* and n^* are used later in this article to construct a pore-size indicator parameter (α^*/n^*) that will prove useful in characterizing dispersion phenomena in terms of a soil's textural properties.

3. Results and Discussion

3.1. Theoretical Dispersion Model

[7] The column tests were carried out under uniform saturation ratio, as discussed earlier. In addition, steady

Table 1. Properties of Selected Porous Media and Estimated Parameters

	Soil Properties		Textural Parameters			Estimated Parameters		
	d_{50} , cm	ρ_s , g cm ⁻³	α^* , cm ⁻¹	n^*	$ r ^a$	α_{100}^b , cm	a^c	b^d
Toyoura sand	0.018	2.65	0.036	4.2	0.86	0.066	0.27	1.68
Glass beads (0.025)	0.025	2.50	0.030	11.8	0.64	0.030	0.83	3.67
Glass beads ^e (0.10)	0.100	0.125	0.80	2.36
Silica sand ^e	0.025	2.71	0.027	4.7	...	0.049	0.51	2.61

^aRegression coefficient.
^bDispersivity under fully saturated condition.
^cScale parameter in $Pe = aSr^b$.
^dShape parameter in $Pe = aSr^b$.
^eHaga et al. [1999].
^fData not reported in the original references.
^gPadilla et al. [1999].

state flow conditions were achieved during the tests by means of a parallel pump that maintained constant inflow and outflow in the column. Under these simplifying conditions, the equation used to describe mass transport in the columns was

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial z} \left[D(\theta, v) \frac{\partial C}{\partial z} \right] - v \frac{\partial C}{\partial z} \tag{2}$$

in which C is the solute concentration, θ is the volumetric water content, $v = q/\theta$ equals the average pore-water velocity (q is the Darcian velocity), z is the vertical coordinate, t is time elapsed since the start of tracer transport in the column, and $D(\theta, v)$ is the dispersion coefficient. An approximate solution of equation (2) for the experimentally applicable initial and boundary conditions is given by the following expression (L is the column length and $p = vt/L$ is the number of pore volumes in the packed column solution first obtained by Ogata and Banks [1961; see also van Genuchten and Parker, 1984]:

$$\frac{C}{C_0} = \frac{1}{2} \left\{ \operatorname{erfc} \left[\frac{1-p}{2\sqrt{D(\theta, v) \frac{p}{vL}}} \right] + \exp \left(\frac{vL}{D(\theta, v)} \right) \operatorname{erfc} \left(\frac{1+p}{2\sqrt{D(\theta, v) \frac{p}{vL}}} \right) \right\} \tag{3}$$

[8] In equation (3), erfc denotes the complementary error function. The relative concentration in the left-hand side of equation (3) denotes the ratio of the Cl^- concentration in the column's effluent (C) to that in the injected tracer (C_0). The solution equation (3) is used in the analysis of experimental breakthrough curves presented below.

3.2. Estimation of the Dispersion Coefficient

[9] The dispersion coefficient was determined by fitting the solution equation (3) to experimental tracer dispersion data from the column tests carried out by the authors. Several regression lines depicting the relationship between the dispersion coefficient and the average pore-water velocity are shown in Figure 5. (The average pore-water velocity was determined from the measured flow rate and the associated water content.) The regression lines indicate a positive linear relationship between the dispersion coefficient

and the average pore-water velocity in the velocity range considered in this study. The regression lines were grouped into ranges of the saturation ratio. It is evident in Figure 5 that there is a clear differentiation in the slope of the fitted regression lines with respect to the saturation ratio: the larger the saturation ratio, the smaller the slope of the regression lines. There were no tracer measurements made for pore-water velocity less than 0.1 cm min⁻¹ due to the predominant role of diffusion at such low velocities.

[10] The results of Figure 5 are in agreement with Scheidegger's [1960] hypothesis of a linear relationship between the dispersion coefficient and the hydraulic gradient, since the average pore-water velocity can be increased by increasing the hydraulic gradient. Yule and Gardner [1978] studied experimentally the relationship between the dispersion coefficient and the pore-water velocity in an unsaturated Plainfield sand. Those authors, however, did not evaluate experimentally the effect of the water content on the dispersion versus water-velocity function. Our experimental results have established that the slope of the regression line between the dispersion coefficient and the average pore-water velocity becomes steeper with decreasing saturation ratio. Figure 5 makes evident that the effect of saturation ratio on the dispersion coefficient for a fixed pore-water velocity is considerable.

3.3. Dispersion Effect on the Breakthrough Curve

[11] Figure 6 shows two breakthrough curves measured in a test column packed with Toyoura sand. Each curve corresponds to a different saturation ratio, and both were obtained with identical pore-water velocities. The continuous lines through the data in Figure 6 are mathematical solutions of the one-dimensional advection-dispersion model (see equation (3)) fitted to experimental tracer data. The data in Figure 6 show that the breakthrough curve rotates clockwise with a decrease in saturation ratio (a similar finding was reported by Krupp and Elrick [1968], Padilla et al. [1999], and Haga et

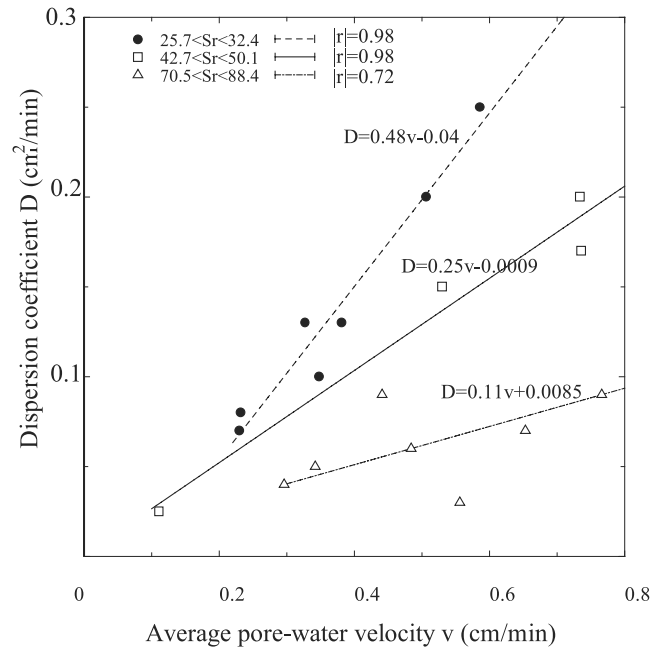


Figure 5. Dispersion coefficient versus average pore-water velocity. The $|r|$ is the regression coefficient.

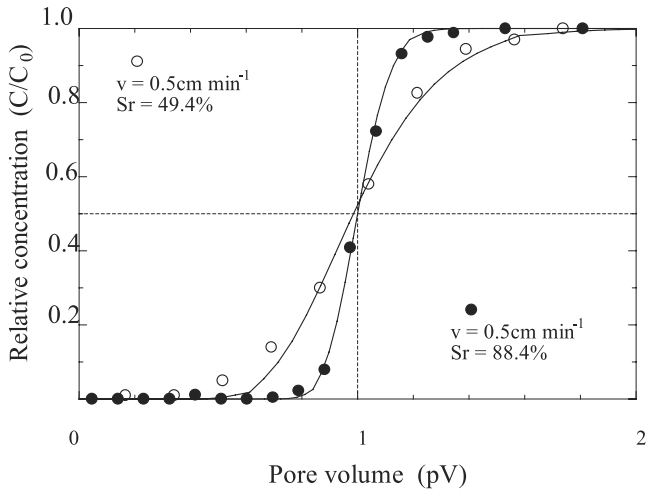


Figure 6. Breakthrough curves for two different saturation ratios.

al. [1999]). Breakthrough took place earlier in the case for which the saturation ratio was 49.4% than in that corresponding to a saturation ratio equal to 88.4%. The number of pore volumes (pV) needed to reach the 1.0 relative concentration becomes larger in the case $S_r = 49.4\%$ than in the case $S_r = 88.4\%$. The latter two features of the breakthrough curves shown in Figure 6 are consistent with the experimental result of increasing dispersion coefficient with decreasing saturation ratio (or water content) for a fixed average pore-water velocity.

3.4. Experimental Estimates of the Peclet Number

[12] The Peclet number was estimated according to its definition $Pe = vd_{50}/D(\theta, v)$, in which d_{50} is the median grain size (taken as a characteristic length of the porous medium in this instance). Following *Haga et al.* [1999], we propose a power function to describe the relationship between the Peclet number and the saturation ratio (S_r) as follows:

$$Pe = aS_r^b \tag{4}$$

in which a and b are fitting parameters. *Haga et al.* [1999] treated a and b as experimental constants. Note that according to equation (4), a and b are scale and shape parameters, respectively, and that a tends to the Peclet number as the saturation ratio approaches one (i.e., $a \rightarrow Pe$ when $S_r \rightarrow 1$). We investigated the validity of equation (4) in Toyoura sand, glass beads, and the silica sand used by *Padilla et al.* [1999], while allowing a and b to depend explicitly on the textural properties of a soil.

[13] A two-step procedure as applied to estimate the scale parameter a that appears in equation (4). First, the dispersivity under fully saturated conditions (α_{100}) was calculated as a function of the ratio α^*/n^* . The results are shown in Figure 7, which shows the fitted regression. The experimental values were well approximated by the fitted regression lines except for the measurements on glass beads (0.025), which fell above the fitted regression line. Next, the fact that a equals the Peclet number at saturation was used to derive the desired function of a versus α^*/n^* :

$$a = \frac{d_{50}}{\alpha_{100}} = \frac{d_{50}}{6.0(\alpha^*/n^*) + 0.015}, \tag{5}$$

which has a regression coefficient $|r| = 0.84$. The empirical expression (5) estimates the Peclet number in terms of (1) the pore-size distribution parameter (n^*), (2) the average pore-size (α^*), and (3) the particle size (d_{50}). Recall that α^* and n^* are the van Genuchten soil-moisture parameters discussed in the context of equation (1). The α^* is related to the average pore size in a porous medium (that is, a larger α^* tends to be associated with a larger average pore size), while n^* is related to the range of pore sizes (i.e., a larger n^* is generally associated with a narrower pore-size range). High values of α^* and n^* generally correspond to sandy soil while fine-textured soils exhibit lower values [*Kool et al.*, 1985]. Equation (5) implies that the scale parameter a , which equals the Peclet number at saturation, increases as the pore-size parameter α^*/n^* increases because the dispersion coefficient D (related to the Peclet number by $Pe = vd_{50}/D$) becomes smaller with increasing α^*/n^* . Empirical relationships between dispersivity and particle size, similar to that implied by equation (5), date back to *Perkins and Johnston* [1963].

[14] The derivation of a relationship between the parameter b (see equation (4)) and a^*/n^* was done in two steps. First, the Peclet number was related experimentally to the saturation ratio in Toyoura sand, glass beads (0.025), glass beads (0.10), and silica sand. Results are shown in Figure 8. Next, regression equations were fitted to the Pe vs. S_r data for each soil type. The regressions are graphed in Figure 8. Finally, those regressions were used in conjunction with equation (5) to estimate b in terms of a^*/n^* . Figure 9 shows that the estimates of the shape parameter b were constant with an average value of about 2.0 except for glass beads (0.025). In the latter instance, the departure from the value $b = 2.0$ is attributed to the poor approximation that equation (5) gives to the dispersivity at saturation for glass beads (0.025), as corroborated in Figure 7. An average shape parameter $b = 2.0$ implies that the Peclet number is proportional to the square of the saturation ratio (by virtue of equation (4)) for a particular soil type. Previous studies of dispersion in partly saturated porous media have treated the Peclet number as a constant.

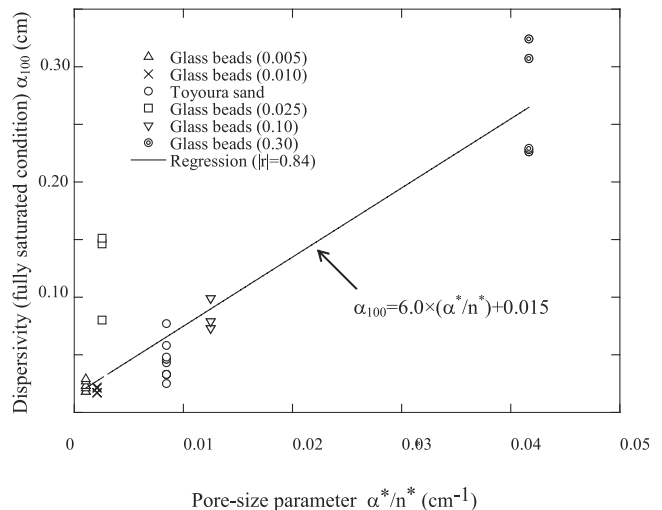


Figure 7. Dispersivity (α_{100} , fully saturated condition) versus pore-size parameter α^*/n^* . The $|r|$ is the regression coefficient.

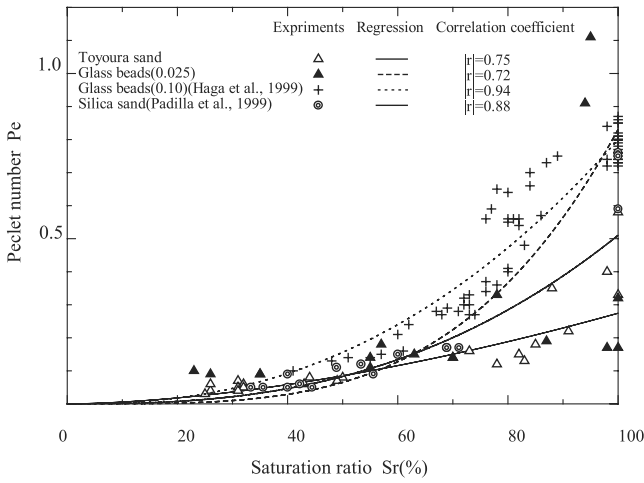


Figure 8. Experimental data, Peclet number (Pe) versus saturation ratio (S_r).

[15] In synthesis, given a soil with specific α^*/n^* parameter, one can infer a and b . From the latter, transport parameters can be inferred, as shown next.

3.5. Dispersivity Estimates

[16] From the definition of the Peclet number $Pe = aS_r^b = vd_{50}/D$ and of the dispersion coefficient $D = \alpha v$ (assuming negligible diffusion), the dispersivity α (in centimeters) can be expressed as follows (in the following equation d_{50} is in centimeters):

$$\alpha = \frac{d_{50}}{aS_r^b} \tag{6}$$

For a given porous medium, the pore-size parameters α^* and n^* can be determined (see Table 1), as well as its median grain size d_{50} (see Table 1). The dispersivity follows

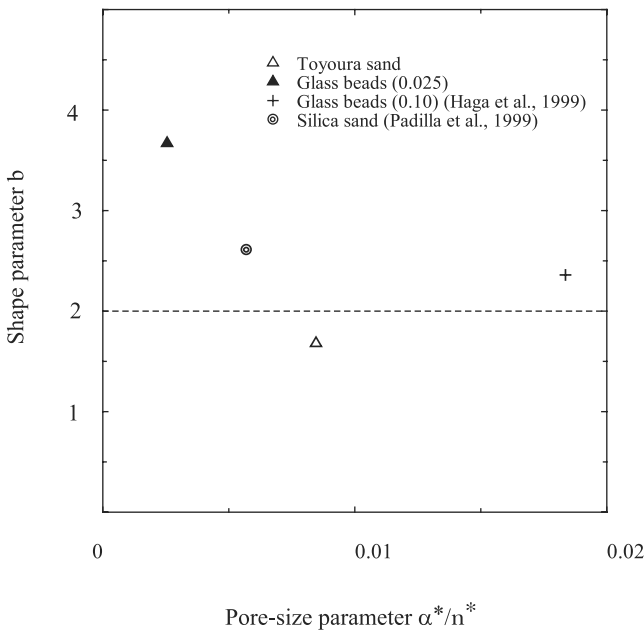


Figure 9. Relationship between the parameter b and the pore-size parameter α^*/n^* .

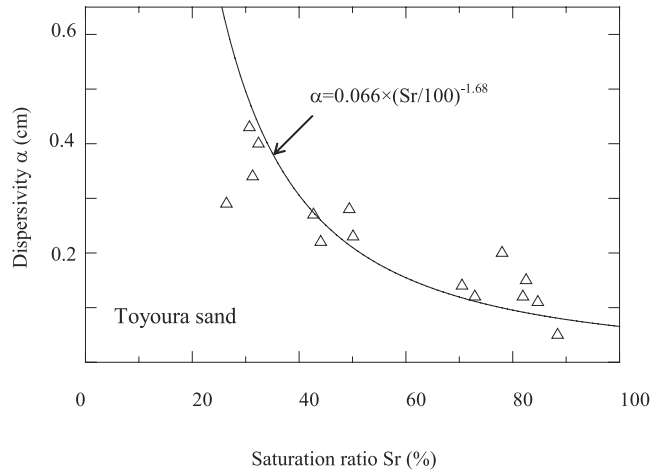


Figure 10. Dispersivity versus saturation ratio in Toyoura sand.

at once from equation (6), given the saturation ratio S_r . Equation (6) was fitted to experimental data pertinent to Toyoura sand, glass beads (0.025), and silica sand [Padilla et al., 1999]. The fitted functions to Toyoura sand, glass beads, and silica sand are shown as smooth lines in Figures 10, 11, and 12, respectively. The data in Figures 10, 11, and 12 were obtained from the various Pe versus S_r experimental results for Toyoura sand and glass beads (0.025) detailed above (see Figure 8) and from the column tests by Padilla et al. [1999], and then expressing the dispersivity as $\alpha = d_{50}/Pe$ for a specific saturation ratio. It is seen in Figures 10, 11, and 12 that the dispersivity tends to decrease with increasing saturation ratio. The power functions fitted to the experimental data except whenever the saturation ratio fell below 50% in glass beads (0.025). This was caused by propagation of error committed in the estimation of α_{100} for glass beads (0.025) (see Figure 7).

[17] The proposed dispersivity equation (6) differs from previous empirical relationships proposed by other investigators. For example, Rumer [1962] proposed a linear

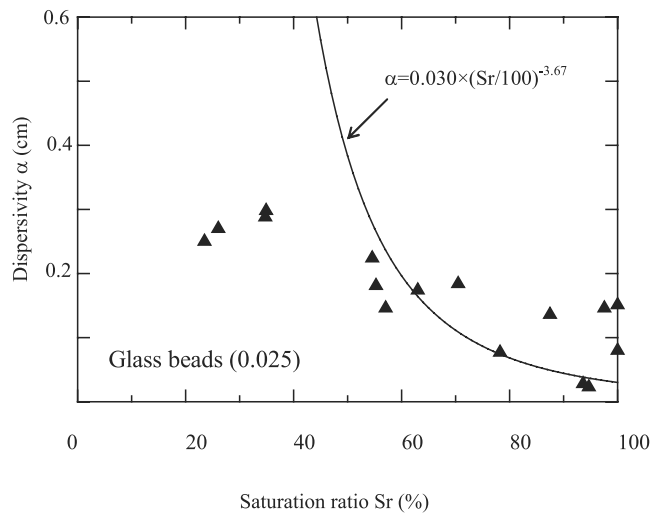


Figure 11. Dispersivity versus saturation ratio in glass beads (0.025).

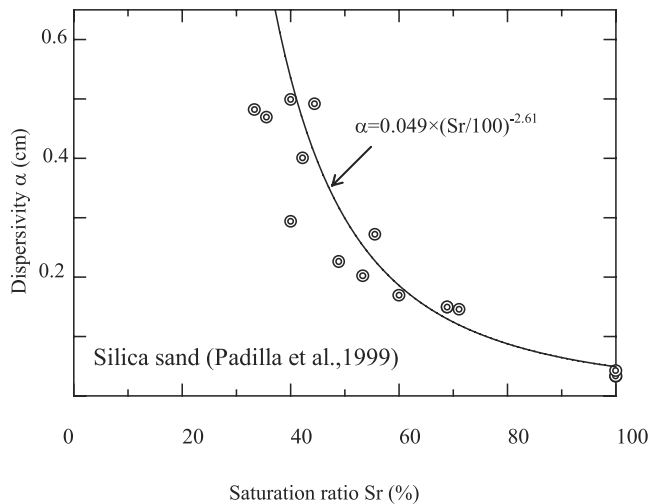


Figure 12. Dispersivity versus saturation ratio in silica sand [Padilla et al., 1999].

relationship between the dispersion coefficient and the average pore-water velocity. The latter author concluded that the proportionality constant (i.e., the dispersivity) depends on the geometry of the porous material. Bresler [1973] considered dispersivity to be an experimental constant that depends on the characteristics of a porous medium. The results of Figures 10, 11, and 12 show that dispersivity is a function of a pore-size parameter (α^*/n^*) and of the saturation ratio.

4. Conclusions

[18] The dispersion coefficient was determined by fitting a one-dimensional advection-dispersion model to experimental tracer data from test columns packed with Toyoura sand or glass beads (0.025). The experimental results quantified the effect of the saturation ratio and pore-water velocity on one-dimensional hydrodynamic dispersion. It is concluded that (1) the dispersion coefficient increases linearly with increasing pore-water velocity for a fixed saturation ratio; (2) the slope of the fitted dispersion versus pore-water velocity regression lines increases with decreasing saturation ratio; (3) the Peclet number is well approximated by a power function of the saturation ratio, $Pe = a S_r^b$, where a and b are empirical constants that are determined from a pore-size parameter derived from the van Genuchten model of water-retention characteristics and particle diameter; (4) the Peclet number decreases with decreasing saturation ratio; (5) the magnitude of the scale parameter a , which equals the Peclet number under fully saturated conditions, increases linearly with increasing pore-size parameter α^*/n^* ; (6) the shape parameter b has an average value of approximately 2.0 irrespective of α^*/n^* ; and (7) the dispersivity in partly saturated media was well approximated by a power function of the saturation ratio, and the fitted function varied with the textural characteristics of a soil.

[19] Our experimental results provide further evidence for the need to consider the effect of water content on the dispersion characteristics of unsaturated porous media. Several quantitative relationships between the dispersion coefficient and the pore-water velocity for a fixed saturation

ratio, and between the dispersivity and the saturation ratio, have been developed in this article.

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